

# Equilibration of quasi-isolated quantum systems

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## Abstract

The evolution of a quasi-isolated finite quantum system from a nonequilibrium initial state is considered. The condition of quasi-isolation allows for the description of the system dynamics on the general basis, without specifying the system details and for arbitrary initial conditions. The influence of surrounding results in (at least partial) equilibration and decoherence. The resulting equilibrium state bears information on initial conditions and is characterized by a representative ensemble. It is shown that the system average information with time does not increase. The partial equilibration and non-increase of average information explain the irreversibility of time.

**Keywords:** Quasi-isolated quantum systems, Equilibration, Decoherence, Average information, Irreversibility of time

# 1 Introduction

The feasibility of producing various kinds of finite quantum systems has sparked recently a strong interest in studying nonequilibrium properties of such objects. As examples of finite systems, it is possible to mention spin assemblies, quantum dots and wells, and trapped atoms. The current studies follow mainly two trends. The first direction, started yet by Schrödinger [1,2], considers thermalization of a *non-isolated* system coupled to a giant thermal reservoir. Related to this is the case of local equilibration, when a finite part of a large system is considered, with the rest of the system playing the role of a giant reservoir. The second track, pioneered by von Neumann [3,4], explores relaxation of *isolated* quantum systems to quasi-stationary states characterized by ergodic averages. The relaxation of composite finite systems also pertains to this track [5-7]. There have appeared a number of papers on these topics of equilibration. Extensive list of literature can be found in the recent review articles [8-13].

The aim of this paper is to study the third way, when a finite quantum system is *quasi-isolated* so that, though there exists some surrounding, but it is such that it does not disturb the system. In mathematical terms, this means that the matrix representation of all operators from the algebra of local observables is not influenced by the presence of the surrounding. It turns out that such quasi-isolated systems enjoy interesting specific properties, essentially differing them from both non-isolated as well as isolated systems.

## 2 Quasi-isolated quantum systems

Let us consider a system described by a Hamiltonian  $H_A$  acting on a Hilbert space  $\mathcal{H}_A$ . And let there exist a surrounding characterized by a Hamiltonian  $H_B$  on a Hilbert space  $\mathcal{H}_B$ . The total Hamiltonian is the sum

$$H_{AB} = H_A + H_B + H_{int} , \quad (1)$$

where  $H_{int}$  is an interaction part. Hamiltonian (1) does not depend on time and acts on the space

$$\mathcal{H}_{AB} = \mathcal{H}_A \otimes \mathcal{H}_B . \quad (2)$$

The system statistical ensemble is the pair  $\{\mathcal{H}_{AB}, \hat{\rho}_{AB}(t)\}$  of space (2) and statistical operator

$$\hat{\rho}_{AB}(t) = \hat{U}_{AB}(t) \hat{\rho}_{AB} \hat{U}_{AB}^\dagger(t) , \quad (3)$$

with the evolution operator

$$\hat{U}_{AB} = \exp(-iH_{AB}t) . \quad (4)$$

Here  $\hat{\rho}_{AB} \equiv \hat{\rho}_{AB}(0)$ . The statistical operator is normalized,  $\text{Tr}_{AB} \hat{\rho}_{AB}(t) = 1$ , where the trace is over space (2).

The quantities of interest are the averages of the operators  $\hat{A}$  from the algebra of local observables acting on the space  $\mathcal{H}_A$ . Such averages correspond to the measurable quantities

$$\langle \hat{A}(t) \rangle \equiv \text{Tr}_{AB} \hat{\rho}_{AB}(t) \hat{A} = \text{Tr}_A \hat{\rho}_A(t) \hat{A} , \quad (5)$$

where

$$\hat{\rho}_A(t) \equiv \text{Tr}_B \hat{\rho}_{AB}(t) . \quad (6)$$

The system, by definition, is quasi-isolated from the environment when the system Hamiltonian is conserved, such that

$$[H_A, H_{AB}] = 0 . \quad (7)$$

As a consequence, we have

$$[H_A, H_B + H_{int}] = [H_A, H_{int}] = 0 .$$

The quasi-isolation condition (7) guarantees that the matrix representation of all system operators from the algebra of local observables remains unchanged in the presence of the environment. In that sense, the latter does not disturb the system. Condition (7) slightly differs from the notion of a nondemolition measurement [14]. According to the latter, a nondemolition measurement of an observable, represented by the operator  $\hat{A}$ , is such that this operator is an integral of motion,  $[\hat{A}, H_{AB}] = 0$ . Particular systems in an environment satisfying Eq. (7) have been considered, assuming that this environment is a bath composed of an infinite number of harmonic oscillators [15-19]. But here, we do not specify the environment. It will be shown below that the quasi-isolation condition (7), as such, is sufficient for deriving the general properties of equilibrating quantum systems.

Let the eigenproblem for  $H_A$  be of the form

$$H_A |n\rangle = E_n |n\rangle . \quad (8)$$

Then, because of commutator (7), the eigenproblem for Hamiltonian (1) reads as

$$H_{AB} |nk\rangle = (E_n + \varepsilon_{nk}) |nk\rangle , \quad (9)$$

where  $|nk\rangle \equiv |n\rangle \otimes |k\rangle$  and  $\varepsilon_{nk}$  is the eigenvalue of the problem

$$(H_B + H_{int}) |nk\rangle = \varepsilon_{nk} |nk\rangle . \quad (10)$$

The quantities of interest are the averages of the operators  $\hat{A}$  from the algebra of local observables acting on the space  $\mathcal{H}_A$ . Such averages correspond to the measurable quantities (5) describing the system behavior. Using the basis composed of the vectors  $|nk\rangle$  gives

$$\langle \hat{A}(t) \rangle = \sum_{mn} \rho_{mn}^A(t) A_{nm} , \quad (11)$$

where  $A_{mn} \equiv \langle m | \hat{A} | n \rangle$ . The reduced density matrix

$$\rho_{mn}^A(t) \equiv \langle m | \hat{\rho}_A(t) | n \rangle = \sum_k \rho_{mnk}(t) \quad (12)$$

is the sum of the terms

$$\rho_{mnk}(t) \equiv \langle mk | \hat{\rho}_{AB}(t) | nk \rangle = \rho_{mnk}(0) \exp\{-i(\omega_{mn} + \varepsilon_{mnk})t\} , \quad (13)$$

with the initial values

$$\rho_{mnk}(0) \equiv \langle mk | \hat{\rho}_{AB}(0) | nk \rangle , \quad (14)$$

and with the transition frequencies

$$\omega_{mn} \equiv E_m - E_n , \quad \varepsilon_{mnk} \equiv \varepsilon_{mk} - \varepsilon_{nk} . \quad (15)$$

As follows from Eqs. (15),

$$\omega_{nn} = 0 , \quad \varepsilon_{nnk} = 0 . \quad (16)$$

Hence the diagonal elements of matrix (12) do not depend on time:

$$\rho_{nn}^A(t) = \sum_k \rho_{nnk}(0) \equiv \rho_{nn}(0) . \quad (17)$$

Then, separating in average (11) the diagonal and nondiagonal terms yields

$$\langle \hat{A}(t) \rangle = \sum_n \rho_{nn}(0) A_{nn} + \sum_{m \neq n} \rho_{mn}^A(t) A_{nm} . \quad (18)$$

The density matrix (12) can be written as

$$\rho_{mn}^A(t) = R_{mn}(t) \exp(-i\omega_{mn}t) , \quad (19)$$

where

$$R_{mn}(t) \equiv \sum_k \rho_{mnk}(0) \exp(-i\varepsilon_{mnk}t) . \quad (20)$$

Introducing the density function

$$g_{mn}(\varepsilon) \equiv \sum_k \rho_{mnk}(0) \delta(\varepsilon - \varepsilon_{mnk}) \quad (21)$$

makes it possible to rewrite Eq. (20) as the integral transformation

$$R_{mn}(t) = \int_{-\infty}^{\infty} g_{mn}(\varepsilon) e^{-i\varepsilon t} d\varepsilon . \quad (22)$$

The density function (21) is normalized so that

$$\int_{-\infty}^{\infty} g_{mn}(\varepsilon) d\varepsilon = \sum_k \rho_{mnk}(0) \equiv \rho_{mn}(0) . \quad (23)$$

This allows us to represent it as

$$g_{mn}(\varepsilon) = \rho_{mn}(0) p_{mn}(\varepsilon) , \quad (24)$$

with the distribution function normalized to one,

$$\int_{-\infty}^{\infty} p_{mn}(\varepsilon) d\varepsilon = 1 . \quad (25)$$

Thence Eq. (20) can be written as

$$R_{mn}(t) = \rho_{mn}(0) D_{mn}(t) , \quad (26)$$

with the *decoherence factor*

$$D_{mn}(t) \equiv \int_{-\infty}^{\infty} p_{mn}(\varepsilon) e^{-i\varepsilon t} d\varepsilon . \quad (27)$$

Consequently, matrix (19) becomes

$$\rho_{mn}^A(t) = \rho_{mn}(t) D_{mn}(t) , \quad (28)$$

where

$$\rho_{mn}(t) \equiv \rho_{mn}(0) \exp(-i\omega_{mn}t) . \quad (29)$$

As a result, for average (18), we have

$$\langle \hat{A}(t) \rangle = \sum_n \rho_{nn}(0) A_{nn} + \sum_{m \neq n} \rho_{mn}(t) A_{nm} D_{mn}(t) . \quad (30)$$

### 3 Possible types of equilibration

If the surrounding is finite, so that the spectrum, defined by eigenproblem (10), is discrete, then the density function (21) is a sum of delta functions. Therefore factor (27) is a sum of exponentials and average (30) is a quasi-periodic function. In such a case, there is no equilibration in the strict sense, as far as any initial value of the observable will be reproduced after the Poincaré recurrence time. However, if the number of degrees of freedom, characterizing the surrounding, is sufficiently large, the recurrence time can be very long [12]. Then the system tends to a quasi-equilibrium state, in which it lives during most of the time in the temporal interval before the recurrence time.

But if the surrounding is so large that can be treated as infinite, then the multi-index  $k$  becomes continuous and the sums over  $k$  are to be replaced by integrals. In that case the density function (21) can be measurable, similarly to the properties of densities of states for large statistical systems. If so, the related state distribution, introduced in Eq. (24), is also measurable. Then the following general statement holds true.

**Theorem 1.** *If the state distribution  $p_{mn}(\varepsilon)$  is measurable, then the quasi-isolated quantum system equilibrates in the strict sense, so that*

$$\lim_{t \rightarrow \infty} \langle \hat{A}(t) \rangle = \sum_n \rho_{nn}(0) A_{nn} . \quad (31)$$

**Proof.** The state distribution, by assumption, is measurable and, by definition (25), it is  $L^1$  integrable. Then, according to the Riemann-Lebesgue lemma [20], for integral (27), one has

$$\lim_{t \rightarrow \infty} D_{mn}(t) = 0 .$$

The matrix  $\rho_{mn}(t)$  depends on time through the bounded function  $\exp(-i\omega_{mn}t)$ . Since, by the Riemann-Lebesgue lemma, the decoherence factor tends to zero, we come to the limiting equality (31).

As an illustration, showing how the density function (21) can become measurable, let us treat the index  $k$  as continuous, so that function (21) be represented by the integral

$$g_{mn}(\varepsilon) = \int \rho_{mnk}(0) \delta(\varepsilon - \varepsilon_{mnk}) d\mu(k) ,$$

with a  $d$ -dimensional differential measure

$$d\mu(k) = \frac{2\pi^{d/2}}{\Gamma(d/2)} k^{d-1} dk ,$$

corresponding to a spherically symmetric surrounding.

The delta-function of a function  $f(x)$  is defined by the expression

$$\delta(f(x)) = \sum_i \frac{\delta(x - x_i)}{|f'(x_i)|} ,$$

in which  $x_i$  are simple zeros given by the equation  $f(x_i) = 0$ , with the derivatives  $f'(x_i)$  being nonzero. Then, for our case, we get

$$\delta(\varepsilon - \varepsilon_{mnk}) = \sum_i \frac{\delta(k - k_i)}{|\varepsilon'_{mnk_i}|} ,$$

where  $k_i = k_{imn}(\varepsilon)$  is defined by the equations

$$\varepsilon - \varepsilon_{mnk_i} = 0 , \quad \varepsilon'_{mnk_i} \equiv \frac{d\varepsilon_{mnk_i}}{dk_i} \neq 0 .$$

This reduces the density function to the measurable form

$$g_{mn}(\varepsilon) = \frac{2\pi^{d/2}}{\Gamma(d/2)} \sum_i \rho_{mnk_i}(0) \frac{k_i^{d-1}}{|\varepsilon'_{mnk_i}|} .$$

The second term in Eq. (30) is caused by quantum coherence. Therefore, its disappearance because of the action of environment, as in limit (31), is named the environment induced decoherence [21-23].

The concrete expression for the decoherence factor (27) is defined by the state distribution  $p_{mn}(\varepsilon)$  induced by surrounding. Keeping in mind a large number of random perturbations, produced by the surrounding, the induced distribution, in view of the central limit theorem, can be modeled by the Gaussian form, with a standard deviation  $\sigma_{mn}$ ,

$$p_{mn}^G(\varepsilon) = \frac{1}{\sqrt{2\pi} \sigma_{mn}} \exp \left( - \frac{\varepsilon^2}{2\sigma_{mn}^2} \right) .$$

As a result, the decoherence factor is also Gaussian

$$D_{mn}^G(t) = \exp \left\{ - \frac{1}{2} (\sigma_{mn} t)^2 \right\} . \quad (32)$$

In the case of the Lorentz distribution

$$p_{mn}^L(\varepsilon) = \frac{\gamma_{mn}}{\pi(\varepsilon^2 + \gamma_{mn}^2)} ,$$

we have the exponential form

$$D_{mn}^L(t) = \exp(-\gamma_{mn}t) . \quad (33)$$

If the induced density is of the Poisson type

$$p_{mn}^P(\varepsilon) = \frac{1}{2\gamma_{mn}} \exp\left(-\frac{|\varepsilon|}{\gamma_{mn}}\right) ,$$

we get the decoherence factor

$$D_{mn}^P(t) = \frac{1}{1 + (\gamma_{mn}t)^2} . \quad (34)$$

When the surrounding is modeled by a uniform distribution

$$p_{mn}^U(\varepsilon) = \frac{1}{2\Delta_{mn}} \Theta(\Delta_{mn} - \varepsilon)\Theta(\Delta_{mn} + \varepsilon) ,$$

the decoherence factor is of power law with oscillations:

$$D_{mn}^U(t) = \frac{\sin(\Delta_{mn}t)}{\Delta_{mn}t} . \quad (35)$$

Under different circumstances, one can meet different behavior of the decoherence factor. For instance, the relaxation to an equilibrium state can be Gaussian [24], or exponential [15,19,25], or of power law [16]. Generally, the influence of surrounding can be represented by a linear combination of the above types of induced densities. Hence, the decoherence factor can also consist of several parts. For example, it can be a combination of the Gaussian and exponential terms [11,17,18]. In any case, if the density  $p_{mn}(\epsilon)$  is measurable, then a quasi-isolated quantum system equilibrates to a stationary state characterized by the diagonal elements  $\rho_n \equiv \rho_{nn}(0)$ , whose definition involves information on the initial state of the system, which needs to be given. The most general method of characterizing a stationary statistical system is by constructing the corresponding representative ensemble by maximizing the system entropy, under prescribed additional constraints [26-28], which is equivalent to the minimization of the information functional [29,30]. One obvious constraint is the normalization of  $\rho_n$ . Other constraints are given by the average values of *constraint operators*  $\hat{C}_i$ , usually corresponding to some observable quantities  $C_i$  and initial conditions [31].

A quasi-isolated quantum system can also thermalize, when on the manifold of initial conditions there exists a basin of attraction, such that limit (31) does not depend on the particular choice of initial conditions from this basin of attraction [12]. A simple case is when the system initial state is an eigenstate, say  $|j\rangle$ , so that  $\rho_{nn}(0) = \delta_{nj}$ , then limit (31) is exactly  $A_{jj}$ . Suppose now that the initial state is prepared such that  $\rho_{nn}(0)$  is nonzero only for a window  $\mathbb{N}_j$  of the indices  $n \in \mathbb{N}_j$  around  $j$ , where the eigenvalue of  $H_A$  in Eq. (8) is  $E_j$ . And let this window be so narrow that  $\Delta A \equiv \max_{n \in \mathbb{N}_j} A_{nn} - \min_{n \in \mathbb{N}_j} A_{nn}$  be much smaller than  $|A_{jj}|$ . Then, by the mean value theorem, the time limit (31) is again  $A_{jj}$  for any normalized  $\rho_{nn}(0)$ . Since this is valid for any normalized distribution, it is possible to take, for simplicity, the uniform expression  $\rho_{nn}(0) = 1/Z_j$ , where  $Z_j$  is the

number of states in  $\mathbb{N}_j$ . This expression corresponds to the microcanonical distribution, with the energy  $E_j$ . Since limit (31) acquires the microcanonical form, one can say that there happens the eigenstate thermalization. For isolated quantum systems, the eigenstate thermalization was suggested as a hypothesis by Deutsch [32] and Srednicki [33]. Here, we have shown that for a quasi-isolated system, with the prescribed initial condition, this is not a hypothesis but a rigorous asymptotic result. Note that the microcanonical distribution is a particular case of the general representative distribution [12,31].

It is possible, in principle, that, in addition to a measurable part of the density  $p_{mn}(\epsilon)$ , there would exist a non-measurable term of the form

$$p_{mn}^F(\epsilon) = \frac{1}{2} \sum_j c_{mnj} [\delta(\epsilon - \alpha_{mnj}) + \delta(\epsilon + \alpha_{mnj})] ,$$

with positive coefficients  $c_{mnj}$  normalized so that the total density be normalized as in Eq. (25). This would yield the appearance in factor (27) of the fluctuating term

$$D_{mn}^F(t) = \sum_j c_{mnj} \cos(\alpha_{mnj}t) . \quad (36)$$

Then, instead of limit (31), we would have the asymptotic expression

$$\langle \hat{A}(t) \rangle \simeq \sum_n \rho_{nn}(0) A_{nn} + \sum_{m \neq n} \rho_{mn}(t) A_{nm} D_{mn}^F(t) , \quad (37)$$

as time tends to infinity. In that case, the system does not equilibrate completely, but only partially, exhibiting permanent fluctuations. Though the temporal average of the latter expression is zero, the fluctuations can be rather strong and their existence may drastically change the system properties, hence these fluctuations cannot be neglected. A physical example of such a situation can be associated with heterophase fluctuations [29,34].

## 4 Irreversibility of time direction

The problem of time irreversibility has attracted great attention (see, e.g., Refs. [21-23,35,36]). Usually, one connects the irreversibility with the behavior of the system thermodynamic characteristics, such as the increase of entropy with time. The Gibbs entropy is known to be constant for isolated systems, because of which the Boltzmann entropy seems to be preferable for considering this problem [37,38].

Another possibility is to consider the average entropy or the average information. The latter is defined as the average of the information content  $\ln \hat{\rho}_{AB}$ ,

$$I(t) \equiv \text{Tr}_{AB} \hat{\rho}_{AB}(t) \ln \hat{\rho}_{AB} , \quad (38)$$

similarly to the definition of the operator averages (5). Then we have the following statement.

**Theorem 2.** *The average information (38) does not increase with time:*

$$I(t) - I(0) \leq 0 . \quad (39)$$



**Proof.** It is straightforward to see that

$$\begin{aligned}\mathrm{Tr}_{AB}\hat{\rho}_{AB}(t)\ln\hat{\rho}_{AB} &= \mathrm{Tr}_{AB}\hat{\rho}_{AB}\hat{U}^+(t)(\ln\hat{\rho}_{AB})\hat{U}(t) = \\ &= \mathrm{Tr}_{AB}\hat{\rho}_{AB}\ln\left[\hat{U}^+(t)\hat{\rho}_{AB}\hat{U}(t)\right] = \mathrm{Tr}_{AB}\hat{\rho}_{AB}\ln\hat{\rho}_{AB}(-t) .\end{aligned}$$

Therefore

$$I(0) - I(t) = \mathrm{Tr}_{AB} [\hat{\rho}_{AB}\ln\hat{\rho}_{AB} - \hat{\rho}_{AB}\ln\hat{\rho}_{AB}(-t)] .$$

Then we use the Gibbs-Klein inequality, proved by Gibbs [39] for classical distributions and generalized by Klein [40] for quantum operators. According to this inequality, for any two non-negative operators  $\hat{A}$  and  $\hat{B}$ , acting on a Hilbert space  $\mathcal{H}$ , one has

$$\mathrm{Tr}_{\mathcal{H}} (\hat{A}\log\hat{A} - \hat{A}\log\hat{B}) \geq \mathrm{Tr}_{\mathcal{H}}(\hat{A} - \hat{B}) .$$

In our case, we get

$$I(0) - I(t) \geq \mathrm{Tr}_{AB} [\hat{\rho}_{AB} - \hat{\rho}_{AB}(-t)] . \quad (40)$$

Since

$$\mathrm{Tr}_{AB}\hat{\rho}_{AB}(-t) = \mathrm{Tr}_{AB}\hat{\rho}_{AB} = 1 ,$$

we come to the sought inequality (39).

The loss of information with time can be interpreted as the origin of the time irreversibility. However, the irreversibility of time is a phenomenon common for all macroscopic systems, whether thermodynamic or generally dynamic. Therefore the explanation of this phenomenon should not be based only on the notion of entropy. Another point of view on the time irreversibility, not necessarily connected with thermodynamics, relies on the fact that, strictly speaking, absolutely isolated systems do not exist, since any given system is always, at least weakly, connected to some surrounding [22,36]. A real system can be quasi-isolated, but cannot be isolated completely, since there always exist small perturbations, often uncontrollable, which induce the interaction of the system with its surrounding [41-43]. This point of view has been emphasized long ago by Borel [44]. Accepting this, we come to the conclusion that any given real system, at least partially, equilibrates, according to Eqs. (31) or (37). The fact that any real system tends to an equilibrated state implies that there exists irreversible evolution, that is, *time is irreversible*. The partially equilibrated state can be a kind of a steady or quasi-steady state [45].

## 5 Conclusion

The main results and conclusions of the present paper can be formulated as follows:

- (i) The temporal evolution of quasi-isolated quantum systems can be treated on the general level, valid for systems of arbitrary physical nature and under any initial conditions.
- (ii) Quasi-isolated systems, with increasing time, equilibrate, at least partially.
- (iii) When the system equilibrates to a stationary state, the latter, generally, keeps information on initial conditions and is characterized by a representative ensemble.

(iv) For some initial conditions, the eigenstate thermalization happens, being a rigorous asymptotic result.

(v) Accepting that all real systems are at the most only quasi-isolated, but never absolutely isolated, defines the arrow of time, explaining why time is irreversible.

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